First principle computation of stripes in cuprates

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We present a first principle computation of vertical stripes in $La_{15/8}Sr_{1/8}CuO_4$ within the LDA+U method. We find that Cu centered stripes are unstable toward O centered stripes. The metallic core of the stripe is quite wide and shows reduced magnetic moments with suppressed antiferromagnetic (AF) interactions. The system can be pictured as alternating metallic and AF two-leg ladders the latter with strong AF interaction and a large spin gap. The Fermi surface shows warping due to interstripe hybridization. The periodicity and amplitude of the warping is in good agreement with angle resolved photoemission experiment. We discuss the connection with low-energy theories of the cuprates.

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Recent theories of the high temperature superconducting cuprates are based on the idea that hole-rich quasi one-dimensional textures (stripes) are the basic building blocs to understand the low-energy physics[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13]. These model computations either assume stripes to obtain a low-energy quantum field theory (QFT)[3, 4, 5, 6, 7, 8, 11, 14] or obtain stripes in simplified model Hamiltonians[1, 2, 9, 10, 12, 13]. For the QFT's detailed information about the symmetry and the extent of real stripes is lacking so much of the modeling is based on guesses and the relevant regimes are identified a posteriori, by confrontation with experiment[15, 16, 17, 18, 19], leading to a plethora of possible scenarios.

In order to constrain low-energy models some progress can be made by solving more or less realistic Hamiltonians in various approximations[1, 9, 12, 13, 20, 21, 22, 23, 24] however these are tight to strong assumptions about the electronic structure since are restricted to a small number of orbitals and/or short range interactions and a single Cu-O plane. Here we present a first principle computation of stripes in cuprates based on the LDA+U method for doping $x = 1/8$ and the experimentally measured magnetic incomensurability $\epsilon = 1/8$. Our computation are based on the full orbital variational space and the three-dimensional Coulomb interaction and so go beyond the previous works. LDA based methods are widely believed to give reliable charge distributions and therefore can provide a realistic picture of stripe textures. We find that a Cu centered solution is not stable. Instead the stripe is O centered and consist of two columns of "metallic" Cu (the core) and two columns of antiferromagnetic (AF) Cu forming an alternating system of metallic and AF two-leg ladders.

Added holes are spread over the "metallic" Cu rows and the surrounding O leading to a stripe core much wider than the traditional stripe picture[16]. The electronic structure consists of a half-filed quasi one-dimensional band for each stripe core corresponding to motion along the stripe. The system can be schematized as an array of one-dimensional electron gases (1DEG) separated by spin-ladders ("the environment" in the language of Ref. [3, 4, 6, 8]) with a large spin-gap. Interstripe hybridization is not negligible but leads to a noticeable warping of the Fermi surface which is in good agreement with angle resolved photoemission experiments[25]. Additionally there is approximate particle-hole symmetry around the Fermi level in good agreement with transport experiments[26, 27]. We provide estimates of the relevant energy scales for "striped" low-energy theories of cuprates.

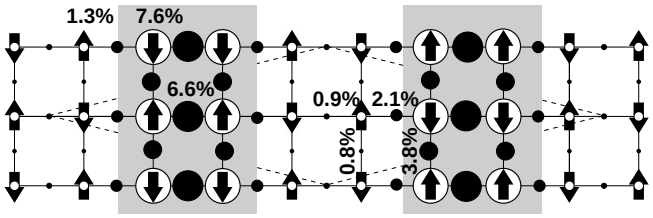

FIG. 1: The hole-charge and spin order within CuO_2 plane. Sites with (without) arrows (indicating spin directions) are Cu (O). The radii of circles are proportional to the hole content inside atomic spheres. The grey regions are metallic core with Cu of type Cu1 and the white regions are the AF ladders with Cu of type Cu2. Numbers indicate the distribution of the doped hole. Not shown are 1,2 % (0,6 %) of hole charge in the apical O's belonging to Cu1 (Cu2) and 0,3 % of charge on La. The unit cell in the CuO_2 plane is shown by the dashed line.

In the present work we used a LDA+U approach[28, 29] realized in frame of scalar relativistic LMTO method within the Atomic Sphere Approximation (ASA)[30] with the Coulomb term of LDA+U functional proposed in Ref. [28]. The radii of atomic

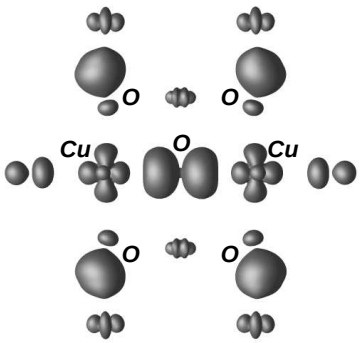

FIG. 2: Wannier function of the active band.

spheres were r(Cu)=2.2 a.u., r(O-plain)=1.94 a.u., r(O-apex)=2.00 a.u., r(La)=3.2 a.u; three types of empty spheres were added. The values of on-cite Coulomb U and exchange J parameters were chosen 8 and 0.88 eV, correspondingly.

We studied a supercell consisted of eight formula units with an additional hole in the absence of the Sr impurity, compensating the charge by adding suitable negative charges to all atoms in the supercell. A Cu centered solution could not be stabilized, not even as a metastable state. In Fig. 1 we show the charge and spin distribution of the stable oxygen centered solution. The hole charge is concentrated on the two core Cu's forming the AF domain wall and the surrounding oxygens (grey region) and leak significantly over the AF regions indicating that interstripe overlap is not negligible as discussed below.

The stripe core consist of rungs of ferromagnetic Cu sites. This locally enhances the effective Cu-Cu hybridization and splits states into the charge transfer band which disperse strongly in the direction of the stripe (Fig. 3). The band crossing the Fermi level (hereafter "the active band"), is half-filled, has quasi one-dimensional character and is similar to the one found in the three-band Hubbard model[12]. The electronic structure is approximately particle-hole symmetric around the chemical potential. This is in agreement with the proposal that approximate particle-hole symmetry in the stripe state is the reason why Hall effect[26, 27] and the thermopower[26] tend to be suppressed in the presence of stripes[5, 12, 27, 31].

A popular model to study the stability and symmetry of stripes in cuprates is the single-band Hubbard model and its strong coupling version, the $t-J$ model[32, 33, 34]. These models are usually derived by considering the low-energy many-body states of a single hole added to the insulator. Zhang and Rice (ZR)[35] pointed out that the hole will occupy a particular linear superposition of the four p oxygen orbitals pointing toward a Cu that has the same symmetry as the Cu $d_{x^2-y^2}$ orbital. The hole in this "ZR-O orbital" and the hole on the Cu form a ZR singlet. The other (orthogonal) combinations of p oxygen orbitals are projected out. By doing so the ZR-O orbital is not allowed to polarize. Such approximation is justified in the dilute limit however when one considers the stability of dense phases special care must be taken on defining low-energy models. In particular for CDW phases, polarization involving high energy states can significantly affect the stability and symmetry[36, 37]. Indeed this problem involves the short range (high energy) physics of the system and the above procedure may be inadequate.

To illustrate the problem we have computed the Wannier function (WF) of the active band (Fig. 2). The WF is centered on the O forming the stripe core but extends considerably to the surrounding oxygens. It is clear that the Cu-centered ZR-O orbitals are strongly polarized and so the usual Hubbard or $t-J$ mapping becomes unreliable. This is in contrast with what was found for one hole added to the AF in LDA+U or inhomogeneous HF where the solution did involve a ZR-O orbital[38, 39]. We conclude that the stability of stripes can not be reliably studied within the $t-J$ or single-band Hubbard model. (Of course the possibility of stripes in those models is a problem of interests in itself but does not have direct experimental relevance). In particular configurations centered in the O will be unfavored since involve a strong O polarization and single band models neglect the relaxation energy involved. If one refrains from studding the stability of stripes one can still assume stripes and use an effective model to describe the low-energy physics.

Coulomb effects (including the polarization effects mention above) produce a splitting of the Madelung potential for a hole in a Cu in the metallic region and a Cu in the AF region of 0.2eV favoring the charge segregation. In LDA this splitting is static but a truly many-body treatment should take into account the dynamical effects of the polarization.

Other parameters are similar to the ones in the dilute limit[40, 41]. i.e. The metallic regions can be described by a two-leg Hubbard model with a hopping along the legs and along the rungs $t_{\parallel}=t_{\perp}=0.52$ eV and a hopping along the diagonals $t'=-0.08$ eV. By treating this model in mean-field with a filling of 3/4 electrons and fitting the gap to the upper bands we obtain $U=4.5$ eV for the Hubbard on-site interaction, similar to the value in the dilute case (~ 5 eV)[40].

The active band is formed by the odd combination of the leg orbitals. The associated Wannier functions are quite different for odd and even combinations, in particular only the odd combination can have admixture with the central p_x orbital as shown in Fig. 2 which shows again that in terms of ZR-O orbitals large relaxations are involved not taken into account in the standard Hubbard model which weights all O's around a Cu on an equal manner.

The two bands immediately below the active one are formed by the orbitals of the AF ladders and are com-

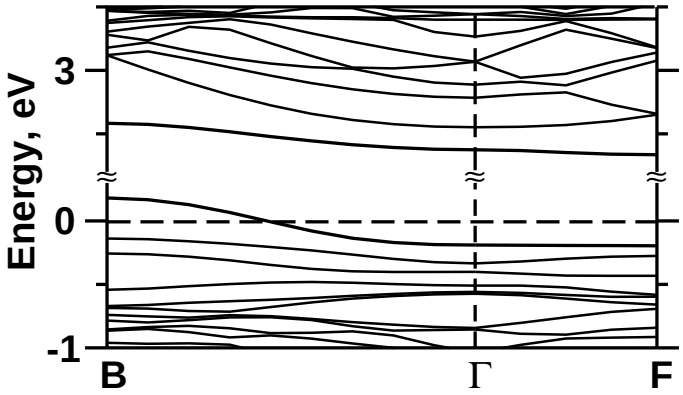

FIG. 3: Calculated band structure of $La_{15/8}Sr_{1/8}CuO_4$ around the Fermi level (E_F=0). Left (right) panel corresponds to the direction parallel (perpendicular) to the stripe. The point B corresponds to momentum $[0, \pi/(2a)]$ in the Cu-O plane.

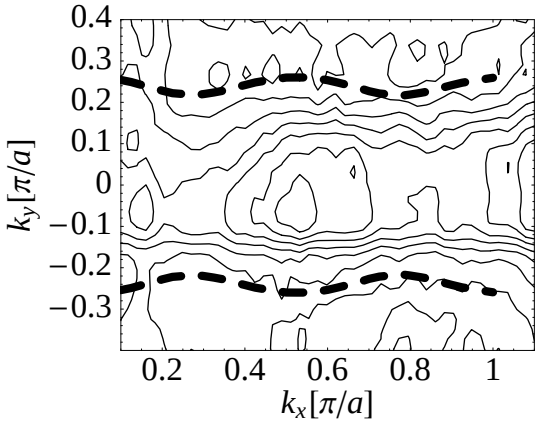

FIG. 4: Angle resolved photoemission spectral weight integrated within 500 meV of the Fermi level, as a function of k_x and k_y[25] together with calculated Fermi surface for 2D CuO_2 plane with stripes oriented along y (dashed line)[47]. Notice that the experimental Fermi surface has contributions due to stripes oriented along y and along x the latter producing the vertical structures at $k_x \sim 0.2\pi/a$.

pletely filled in agreement with the assumption that the environment is an insulator[3, 4, 6, 8]. Therefore the AF regions can be viewed as AF ladders. We computed the magnetic interaction parameters according to prescription of Ref. [42]. The interaction along the rungs, $J_\perp = 146$ meV, results to be enhanced respect to the value obtained by doing the same computation in the stoichiometric system $J = 109$ meV[41] whereas the interaction along the legs, $J_\parallel = 78$ meV, is slightly reduced. If one consider the leg isolated from the 1DEG this would lead to a large spin gap of order ~ 95 meV[43].

Coming back to the metallic regions, it is believed that transverse hopping will drive an array of 1DEG to a two dimensional Fermi liquid or an ordered state[45]. However according to Ref. [3, 4, 5, 8] when one couples the magnetic system and the 1DEG a spin gap will be induced in the 1DEG. This effect will block the effective transverse hopping but not the pair hopping[3, 5, 8]. The system can become a sliding Luttinger phase and eventually a superconductor. Other related scenarios include a boson-fermion model where the bosons are composed fermions coupled antiferromagnetically in the insulating regions[14] and a phase with bond order but with two-dimensional fermions[9, 10]. The large values of the AF interaction in the insulating regions favor all these scenarios. However to make more progress an estimate of the hybridization perpendicular to the stripes is essential.

The crossing of the active band in the Γ-B direction in Fig. 3 does not occur exactly at the middle point (as would be the case for a perfectly half-filled one-dimensional band) but is shifted to the B point. This shift depends on the momentum perpendicular to the stripe and is precisely due to interstripe hopping. i.e holes from the core of one stripe can tunnel to the next stripe through the AF insulating like region. As a result the Fermi surface is not flat but it warps as shown in Fig. 4. Interestingly this explains oscillations exhibit on the experimental Fermi surface in the presence of stripes[25]. In Fig. 4 we show the experimental and the theoretical data. The amplitude and the periodicity of the wrapping is in good agreement with experiment. The large Fermi surface encounter at larger doping has been shown to be in agreement with LDA[44]. The present result shows that in underdoped materials LDA based methods can also predict the Fermi surface including fine details.

The Fermi surface wrapping can be modeled by adding an effective hybridization $t_{\perp,\text{eff}}$ from core to core to the effective two-leg Hubbard model mention above. This gives a contribution to the single electron dispersion of the form $-2t_{\perp,\text{eff}} \cos(4akx)$ with $t_{\perp,\text{eff}} = 0.015$ eV. Notice that this effect does not break the approximate particle-hole symmetry of the system relevant for transport experiments. The effective hybridization at the Fermi surface will be of course renormalized by many-body effects of the kind considered in Ref. [3, 5, 8] which will tend to suppress it or hopping with spin-wave fluctuations[46] which will tend to enhance it. The fact that the wrapping observed is close to the experimental one shows that our estimate is not far from the final value although one should take into account that the experiment is not done strictly at zero energy but integrating in a finite window. More theoretical work is needed to decide the nature of the ground state with this value of the transverse hopping.

To conclude we have presented an LDA+U study of vertical stripe in cuprates. Stripes result to be bond-centered and quite wide in contrast with the traditional stripe picture[16]. The electronic structure shows ap-

proximate particle-hole symmetry around the Fermi level in good agreement with the picture deduced from transport experiments[26, 27]. The system can be pictured as alternating metallic Hubbard and insulating Heisenberg ladders. O polarization effects are important and, at the static level, they contribute to a large Madelung potential splitting between insulating and metallic regions. The dynamical consequences should be further explored. A large exchange interaction in the insulating regions favor mechanisms for superconductivity based on preformed AF singlets which can induce superconductivity on the metallic regions. A non-negligibly hopping transverse from stripe to stripe exist which produces observable effects and is at the core of the low-energy QFT theories. This produces wrapping of the Fermi surface which is in agreement with experimental observation. We believe numerical studies of simplified models taking into account these ingredients should shed light on the problem of superconductivity.

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neighboring CuO_2 layers whereas experimentally they are staked perpendicularly. This produced an unreliable c axis hibrydization. The effect on the Fermi surface was minimized by taking a cut of the three-dimensional Fermi-surface in a plane where the c-hybridization vanish.